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Studies in the Theory of the Generalized Density Operators
I. Foundations

J. J. BRANDSTATTER AND C. PELTZER

Stanford Research Institute, Menlo Park, California

Submitted by Richard Bellman

1. INTRODUCTION

The hierarchy of generalized density operators D^p (or briefly g.d.o.) ($p = 1, 2, \cdots, n$) associated with a quantum mechanical system of n particles were first discussed extensively by Löwdin in 1955 [1] and two valuable reviews of their formal mathematical properties have appeared recently [2, 3]. But some important properties of the g.d.o.'s seem to have been overlooked and the scope of the conceptual and computational implications of their rich mathematical structure does not appear to have been fully realized by most physicists. Our aim here is to give a systematic development of their theory which will provide a sound basis for further theoretical studies of many-body problems and for applications of these concepts to solid state physics and quantum chemistry. Particular emphasis will be placed on precise definitions of the spaces and operators introduced and on a rigorous mathematical development, heuristic arguments being invoked only in the physical interpretation of certain results and methods. Only in this way do we believe that significant progress can be achieved both conceptually and quantitatively in most many-body problems facing us presently.

2. PRELIMINARIES

We consider a quantum mechanical system of n particles (n fixed) and denote by x_i ($i = 1, 2, \cdots, n$) the configuration coordinates (spatial and spin) of the ith particle, by $\mathscr{E}_i$ and $\mathscr{H}_i$ the associated one-particle configuration and state spaces.

DEFINITION 1. *The configuration space $\mathscr{E}_{(p)}$ of a p-particle system ($p = 1, 2, \cdots, n$) is the direct product of the p one-particle configuration spaces $\mathscr{E}_i$ and the measure $\mu_{(p)}$ is the product measure of the measures μ_i on the $\mathscr{E}_i$'s.*

$$\mathscr{E}_{(p)} = \mathscr{E}_1 \times \mathscr{E}_2 \times \cdots \times \mathscr{E}_p\,, \quad \mu_{(p)} = \mu_1 \times \mu_2 \times \cdots \times \mu_p\,, \quad (p = 1, 2, \cdots, n).$$

DEFINITION 2. *The state space $\mathscr{H}_{(p)}$ of a p-particle system* ($p = 1, 2, \cdots, n$) *is the L^2-space of all complex valued, Lebesgue square integrable functions $\Phi^{(p)}(x_1, \cdots, x_p)$ defined on $\mathscr{E}_{(p)}$, i.e., $\Phi^{(p)} \in \mathscr{H}_{(p)}$ if and only if*

$$\int |\Phi^{(p)}|^2 \, d\mu_{(p)} < \infty.$$

With the inner product defined by

$$(\Phi^{(p)}, \Psi^{(p)}) = \int \Phi^{(p)} \overline{\Psi}^{(p)} d\mu_{(p)} \tag{1}$$

these spaces $\mathscr{H}_{(p)}$ are separable, infinite dimensional Hilbert spaces.

The following theorem is well known, if seldom properly proved in quantum mechanics, and with its generalization (Theorem 2), it is the basic representation theorem for many-particle wave functions.

THEOREM 1 (Orbital representation theorem). *If $\{u_k(x_i)\}$ ($i = 1, 2, \cdots, n$) are any n complete orthonormal* (c.o.n.) *bases for $\mathscr{H}_1, \cdots, \mathscr{H}_n$, then a* c.o.n. *basis for $\mathscr{H}_{(n)}$ is given by the set:*

$$\{e_{(k)_n}(x_1, \cdots, x_n) \equiv u_{k_1}(x_1) \cdots u_{k_n}(x_n)\} \tag{2}$$

with $(k)_n = (k_1, k_2, \cdots, k_n)$ and $(k_\ell = 1, 2, \cdots, \infty; \ell = 1, 2, \cdots, n)$. A proof can be found, e.g., in G. Hellwig [4], *and of course the theorem holds for any $\mathscr{H}_{(p)}$ ($p = 1, 2, \cdots, n$).*

THEOREM 2 (Basis representation theorem). *If*

$$\{f_{k_1}^{(p_1)}(x_1 \cdots x_{p_1})\}, \quad \{f_{k_2}^{(p_2)}(x_{p_1+1}, \cdots, x_{p_1+p_2})\}, \quad \cdots, \quad \{f_{k_s}^{(p_s)}(x_{p_s+1}, \cdots, x_n)\}$$

are any s c.o.n. *bases for $\mathscr{H}_{(p_1)}, \cdots, \mathscr{H}_{(p_s)}$ with $\sum_{\ell=1}^{s} p_\ell = n$, then a* c.o.n. *basis for $\mathscr{H}_{(n)}$ is given by the set*

$$\{e_{(k_1,\ldots,k_s)}(x_1, \cdots, x_n) \equiv f_{k_1}^{p_1}(x_1, \cdots, x_{p_1}) \cdots f_{k_s}^{p_s}(x_{p_{s-1}+1}, \cdots, x_n)\} \tag{3}$$

Making use of Theorem 1, the proof is immediate in view of the definition and properties of $\mathscr{E}_{(n)}$ and $\mathscr{H}_{(n)}$, in particular of the product nature of the measure $\mu_{(n)}$. One should note that Theorem 2 contains in particular the geminal representation (in terms of 2-particle wave functions if n is even, 2-particle wave functions and one 1-particle wave function if n is odd).

The further characterization of the state spaces and observables of systems of identical particles will be considered only in the next paper where certain specific aspects of the g.d.o. theory of such systems will be discussed.

3. Completely Continuous Operators—The Cross Operator

The class of completely continuous operators in Hilbert spaces is of particular interest not only because of its rich mathematical structure but also here because many operators of quantum mechanics belong to it. Since its theory appears to be rather unfamiliar to many physicists, we shall give a brief outline of some essential definitions and properties, referring the reader to Refs. 5-8 for proofs and further elaboration. As these studies will repeatedly illustrate, the recognition of the complete continuity of an operator not only allows one to obtain directly many spectral properties and representations, but also leads one naturally to some of the powerful approximation methods of functional analysis.

Definition 3. *An operator*[1] *T, mapping a Hilbert space $\mathscr{H}_1$ into a Hilbert space $\mathscr{H}_2$, $T : \mathscr{H}_1 \to \mathscr{H}_2$, is called completely continuous (or briefly cc) if for every bounded sequence of elements $\{f_i\}$ of $\mathscr{H}_1$, the transformed sequence $\{Tf_i\}$ contains a strongly convergent subsequence (to an element in $\mathscr{H}_2$).*

There exists several other equivalent definitions of *cc* operators in a Hilbert space; in particular the following one which will be stated as

Lemma 1. *An operator T is cc* iff *there exists a sequence of finite rank operators (i.e., an operator whose range is finite dimensional),*

$$\{T_n\}\ (n = 1, 2, \cdots) \qquad \textit{such that} \qquad \| T - T_n \| \to 0 \qquad \text{(see Ref. 6).}$$

The significance of this lemma for approximation purposes is obvious and it underlies general approximation methods such as the method of moments, etc.

As an example of a *cc* operator, we introduce the cross operator[6] defined by:

Definition 4. *Let f and g be any two elements of the Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$, respectively. The cross operator $(g \otimes f)$ is given by*

$$(g \otimes f)\, h = (h, f)\, g \qquad \textit{for every} \qquad h \in \mathscr{H}_1 . \tag{4}$$

One can easily show that this operator is a *cc* mapping of $\mathscr{H}_1$ into $\mathscr{H}_2$ and its particular usefulness in the present context is a reflection of the intrinsic tensor product nature of the state spaces. (See following papers.)

Among others, one should note the following properties of *cc* operators:

(i) They are bounded and possess a (unique) adjoint T^*, also *cc*.

[1] All operators considered are assumed linear.

(ii) The products AT and TA of a *cc* operator T by a bounded linear operator A are *cc*, as is any finite linear combination of *cc* operators.

(iii) Every finite rank operator is *cc.*

(iv) *cc* operators defined everywhere on an *infinite* dimensional Hilbert space possess *no* inverse.

In the sequel, we shall make use of three basic theorems on *cc* operators:

THEOREM 3 (Polar decomposition)[2]. *If T is a cc operator mapping $\mathscr{H}_1$ into $\mathscr{H}_2$, then T is of the form $T = W[T]$ where $[T] = (T^*T)^{1/2}$ and W is a partially isometric operator of domain $\mathscr{H}_1$ and range in $\mathscr{H}_2$. This "polar decomposition" is unique, except that if T is of finite rank, W is unitary but no longer unique.*

THEOREM 4 (Polar representation). *Let $\{f_i\}$ and $\{g_i\}$ be two* o.n. *sets of elements in $\mathscr{H}_1$ and $\mathscr{H}_2$ and $\{\mu_i\}$ be a sequence of real positive numbers, converging to* 0 *if infinite. Then a bounded operator T is cc* iff *it has a "polar representation":*

$$T = \sum_i \mu_i(g_i \otimes f_i) \tag{5}$$

The $\{\mu_i\}$ are the nonzero proper values of $[T]$ and each appears as many times as its (finite) multiplicity; the $\{f_i\}$'s are the corresponding proper functions of $[T]$ and the g_i's are given by $Tf_i = \mu_i g_i$ (or $g_i = Wf_i$).

These two theorems not only *contain* the Sasaki theorems [9], but also show *how* to *construct* the polar representation of a given *cc* operator. If every operator on a finite dimensional space has at least one proper value, this is in no way the case for operators in infinite dimensional spaces, not even for *cc* ones, although every *cc* operator T possesses at least one invariant subspace.[3] But to every *cc symmetric* operator T on a Hilbert space $\mathscr{H}$ corresponds a basis whose elements are proper vectors of T as shown by the next theorem.

THEOREM 5 (Characterization of *cc* symmetric operators). *Every cc symmetric operator T on $\mathscr{H}$ admits a* c.o.n. *set of proper vectors. Its nonzero (real) proper values λ_i are of finite multiplicity and form a sequence converging to zero if infinite. If $\{\varphi_i\}$ is the set of corresponding functions ($T\varphi_i = \lambda_i\varphi_i$, $\lambda_i \neq 0$), then T has the representation:*

$$T = \sum_i \lambda_i(\varphi_i \otimes \bar{\varphi}_i), \tag{6}$$

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[2] This theorem holds for any linear, bounded operator.

[3] An invariant subspace M of an operator T in $\mathscr{H}$ is a proper subspace $\{0\} \neq M \neq \mathscr{H}$ such that $T(M) \subset M$.

where every λ_i appears as many times as its multiplicity. Conversely, every operator defined by (6) is a cc symmetric operator with the λ_i's and φ_i's having the stated properties.

One should note that zero can be a proper value of T of infinite multiplicity; furthermore, if zero is a proper value, then the set $\{\varphi_i\}$ is not complete in $\mathscr{H}$, but it is complete in the range of T; i.e., every vector Tf, $f \in \mathscr{H}$, can be expanded in terms of the $\{\varphi_i\}$:

$$Tf = \sum_i (f, \varphi_i) \varphi_i . \tag{7}$$

The class of all *cc* operators on a Hilbert space $\mathscr{H}$ denoted by (*cc*), forms a Banach space (complete normed space) if the metric adopted is the usual operator norm $\| T \|$, with

$$\| T \| = \operatorname*{Sup}_i \mu_i .$$

There exists two important subclasses of *cc* operators, namely the Hilbert-Schmidt class (σc) which is the set of all *cc* operators such that the squares of the (positive) proper values μ_i of $[T]$ form a convergent series and the trace class (τc), the set of all *cc* operators such that the μ_i's themselves form a convergent series. One easily sees that the trace class is properly contained in the Schmidt class which is itself properly contained in the class of *cc* operators since

$$\sum_i \mu_i \underset{(\tau c)}{<} \infty \Rightarrow \sum_i \mu_i^2 \underset{(\sigma c)}{<} \infty \Rightarrow \mu_i \underset{(cc)}{\rightarrow} 0,$$

while the converse statements are false.

These two subclasses[4] are themselves Banach spaces, with metrics defined by the resp ective norms:

$$\| T \|_\sigma = \Big[\sum_i \| Tf_n \|^2\Big]^{1/2} = \Big[\sum_i \mu_i^2\Big]^{1/2} \qquad \text{(Schmidt norm)} \tag{8}$$

$$\| T \|_\tau = \text{Trace } T = \sum_i \mu_i \qquad \text{(trace norm).} \tag{9}$$

An important property for computational purposes is that in each of these spaces, the set of all finite rank operators is a dense subset, i.e., that every operator of these spaces can be *approximated arbitrarily* closely in the appropriate metric by a finite rank operator[5] (see Lemma 1). (The trace class can

[4] They can actually be turned into Hilbert spaces, by introducing an appropriate inner product.

[5] A detailed discussion of these questions is given in Refs. 6 and 7.

also be defined equivalently as the set of all products of two operators of the Schmidt class.)

4. The Ψ-Mappings

In this section, we shall consider the mappings induced by a wave function $\Psi \in \mathscr{H}_{(n)}$. This preliminary study allows a much deeper understanding of the nature of the generalized density operators and leads in particular in an elegant and natural way to some of their essential properties and representations. For convenience, we use the collective symbols $x \equiv (x_1, x_2, \cdots, x_p)$, $y \equiv (x_{p+1}, \cdots, x_n)$, $x' \equiv (x_1', \cdots, x_p')$, and $y' \equiv (x_{p+1}', \cdots, x_n')$, $dx \equiv d\mu_{(p)}$, $dy \equiv d\mu_{(q)}$, $dx\,dy \equiv d\mu_{(n)}$.

If p and q are any two integers such that $p + q = n$, $\mathscr{E}_{(n)}$ can be decomposed as the direct product $\mathscr{E}_{(p)} \times \mathscr{E}_{(q)}$ with $\mu_{(n)} = \mu_{(p)}\mu_{(q)}$; furthermore, integrals over elements of $\mathscr{E}_{(n)}$, $\mathscr{E}_{(q)}$, $\cdots$ are independent of the order of the successive integrations since product measures are always used here.

Every wave function $\Psi(x, y)$, viewed as defined on the direct product $\mathscr{E}_{(p)} \times \mathscr{E}_{(q)}$, defines two linear mappings $T_p{}^q$ and $T_q{}^p$ between the p- and q-particle state spaces $\mathscr{H}_{(p)}$ and $\mathscr{H}_{(q)}$ by

$$T_p{}^q f(x) = \int \Psi(x, y) f(x)\, dx = \text{element in } \mathscr{H}_{(q)} \tag{10}$$

and

$$T_q{}^p g(y) = \int \Psi(x, y) g(y)\, dy = \text{element in } \mathscr{H}_{(p)}, \tag{10'}$$

where $f(x)$ and $g(y)$ denote respectively any element in $\mathscr{H}_{(p)}$ and $\mathscr{H}_{(q)}$.

Theorem 6. *The Ψ-mappings $T_p{}^q$ (resp. $T_q{}^p$) associated with the n-particle wave function $\Psi(x, y)$ are cc mappings of all of $\mathscr{H}_{(p)}$ (resp. $\mathscr{H}_{(q)}$) into $\mathscr{H}_{(q)}$ (resp. $\mathscr{H}_{(p)}$), and hence are bounded.* (Proof: see Mikhlin [12, p. 49 ff.])

We then have from the general theorems of the preceding section:

Corollary 1. *The Ψ-mapping $T_p{}^q$ admits the polar representation*

$$T_p{}^q = \sum_i \mu_i^{(p)} (g_i^{(q)} \otimes f_i^{(p)}), \tag{11}$$

where the (real) numbers $\mu_i^{(p)}$ are the proper values of $[T_p{}^q] = (T_p^{q*} T_p{}^q)^{1/2}$ and $\{f_i^{(p)}\}$ the o.n. *set of the associated proper functions; furthermore, the $g_i^{(q)}$'s are given by*

$$T_p{}^q f_i^{(p)} = \mu_i^{(p)} g_i^{(q)} \tag{12}$$

and form an o.n. *set in $\mathscr{H}_{(q)}$. A similar result holds for $T_q{}^p$.*

COROLLARY 2. *The Ψ-mapping $T_p{}^q$ belongs to the Schmidt class (σc) since*

$$\left\| T_p{}^q \right\|_\sigma^2 = \sum_i (\mu_i^{(p)})^2 = \int | \Psi(x, y) |^2 \, dx \, dy < \infty \ (= 1 \textit{ if } \Psi \textit{ is normalized})$$

(similarly for $T_q{}^p$).

Another important result is given by:

THEOREM 7 (Kernel representation theorem).[6] *The wave function $\Psi(x, y)$ admits the representation*

$$\Psi(x, y) = \sum_i \mu_i^{(p)} g_i^{(q)}(y) f_i^{(p)}(x). \tag{13}$$

Furthermore this representation is unique in the following sense: the $\mu_i^{(p)}$ are necessarily the (real positive) proper values of $[T_p{}^q]$; $\{f_i^{(p)}\}$ is the o.n. set of associated proper functions (defined uniquely up to a unitary transformation) and the g_i's are given by $T_p{}^q f_i^{(p)} = \mu_i^{(p)} g_i^{(q)}$.

PROOF. (See Schatten).

This representation theorem should not be confused with the general representation Theorem 2; there the sets $\{f_i\}$, $\{g_i\}$ were c.o.n. sets in $\mathscr{H}_{(p)}$ and $\mathscr{H}_{(q)}$ and the representation obtained held for any Ψ in $\mathscr{H}_{(n)}$; here the $\{f_i^{(p)}\}$, $\{g_i^{(q)}\}$ are o.n. but not necessarily complete sets and will be different for different Ψ's.

Theorem 7 apparently gives rise to two representations for Ψ in terms of the proper functions of $[T_p{}^q]$ and $[T_q{}^p]$, but actually these two representations are identical as shown by the following theorem.

THEOREM 8 (Duality). *Let $T_p{}^q$ and $T_q{}^p$ be the Ψ-mappings defined by (10) and $\{\mu_i^{(p)}\}$, $\{\mu_i^{(q)}\}$ be the sets of nonzero proper values of $[T_p{}^q]$ and $[T_q{}^p]$; then, the polar representation of $T_p{}^q$ is*

$$T_p{}^q = \sum_i \mu_i^{(p)} (g_i^{(q)} \otimes f_i^{(p)}),$$

and implies the following "duality relations,"

$$T_p{}^q f_i^{(p)} = \mu_i^{(p)} g_i^{(q)} \tag{12}$$

$$T_q{}^p \bar{g}_i^{(q)} = \mu_i^{(q)} f_i^{(p)} \tag{12'}$$

[6] Part of the results contained in Theorems 7 and 13 are essentially due to E. Schmidt [*Math. Ann.* **63** (1907), 433] and first noticed in this context by B. C. Carlson and J. M. Keller [*Phys. Rev.* **121** (1961), 659].

Furthermore, the sets $\{\mu_i{}^p\}$ and $\{\mu_i{}^q)$ are identical, i.e., $[T_p{}^q]$ and $[T_q{}^p]$ have the same nonzero proper values with the same (finite) multiplicity, and the polar representation of $T_q{}^p$ is given by

$$T_q{}^p = \sum_i \mu_i{}^q(f_i^{(p)} \otimes g_i^{(q)}) \tag{11'}$$

with

$$\mu_i^{(q)} = \mu_i^{(p)} = \mu_i \,. \tag{14}$$

PROOF. (12) follows from Corollary 1, i.e., from the polar representation theorem. Making use of the kernel representation (13), we obtain for $T_q{}^p$ from its definition (10′):

$$T_q{}^p g(y) = \int \Psi(x, y) g(y)\, dy = \sum_i \mu_i^{(p)} f_i^{(p)}(x) \int g_i^{(q)}(y) g(y)\, dy$$

$$= \sum_i \mu_i^{(p)}(g, \bar{g}_i^{(q)}) f_i \qquad \text{for every} \qquad g \in \mathscr{H}_{(q)} \,.$$

Hence

$$T_q{}^p = \sum_i \mu_i^{(p)}(f_i^{(p)} \otimes g_i^{(q)}),$$

proving (11′) because since the polar representation is unique (Theorem 4), the $\mu_i^{(p)}$ must be the nonzero proper values of $[T_q{}^p]$, i.e., identical to the $\mu_i^{(q)}$'s including multiplicity. (12′) follows from (11′) by setting $g = \bar{g}_j^{(q)}$ $(j = 1, 2, \cdots)$.

If we consider now the Ψ-mappings associated with the complex conjugate of Ψ, $\overline{\Psi}(x, y)$, we have similarly:

$$\bar{T}_p{}^q f(x) = \int \overline{\Psi}(x, y) f(x)\, dx, \qquad \bar{T}_q{}^p q(y) = \int \overline{\Psi}(x, y) g(y)\, dy$$

$$\overline{\Psi}(x, y) = \sum_i \mu_i^{(p)} \bar{g}_i^{(q)}(y) f_i^{(p)}(x)$$

$$\bar{T}_p{}^q = \sum_i \mu_i^{(p)}(\bar{g}_i^{(q)} \otimes f_i^{(p)}), \qquad \bar{T}_q{}^p = \sum_i \mu_i^{(p)}(f_i^{(p)} \otimes \bar{g}_i^{(q)})$$

with the same (real) μ_i's.

The next theorem will be essential for our later developments.

THEOREM 9. *The (unique) adjoints of $T_p{}^q$ and $T_q{}^p$ are given by*

$$(T_p{}^q)^* = \bar{T}_q{}^p \qquad \text{and} \qquad (T_q{}^p)^* = \bar{T}_p{}^q. \tag{15}$$

PROOF. Since the Ψ-mappings are linear and bounded, they each possess a unique adjoint. Making use of the polar representation (11), we then obtain

$$(T_p{}^q)^* = \sum_i \bar{\mu}_i^{(p)}(f_i^{(p)} \otimes \bar{g}_i^{(q)}) = \sum_i \mu_i^{(p)}(f_i^{(p)} \otimes \bar{g}_i^{(q)}) = \bar{T}_q{}^p$$

since the μ_i's are real.

5. The Generalized Density Operators

In the preceding section, we have seen that $\Psi(x, y)$, regarded as the kernel of an integral operator, defines two *cc* mappings $T_p{}^q$ and $T_q{}^p$ between the p- and q-particle spaces, and we have also derived in this way an important representation of Ψ, (13). Here we shall consider the hierarchy of generalized density operators D^p of domain and range in $\mathscr{H}_{(p)}$, $(p = 1, 2, \cdots, n)$ and obtain their essential properties very directly from those of the Ψ-mappings.

Considering, for fixed (x, x'), $\Psi(x, y)$ and $\overline{\Psi}(x,' y)$ as elements in $\mathscr{H}_{(q)}$, the integral

$$D^p(x, x') = \int \Psi(x, y) \overline{\Psi}(x', y)\, dy, \qquad (p = 1, 2, \cdots, n) \tag{16}$$

defines a kernel on the direct product space $\mathscr{E}_{(p)} \times \mathscr{E}_{(p')}$ and hence an integral operator D^p of domain and range in $\mathscr{H}_{(p)}$. Since it is obvious from its definition that the kernel $D^p(x, x')$ is *bounded* and *Hermitian*, i.e., $D^p(x, x') = \overline{D^p(x', x)}$, the following definition is justified:

DEFINITION 6. *The "pth order density operator D^p" associated with the wave function $\Psi(x, y) \in \mathscr{H}_{(n)}$ is the operator D^p defined everywhere in $\mathscr{H}_{(p)}$ by the kernel $D^p(x, x')$, i.e.,*

$$D^p f(x) = \int D^p(x, x') f(x')\, dx'$$

$$= \iint \Psi(x, y) \overline{\Psi}(x', y) f(x')\, dx'\, dy, \qquad (p = 1, 2, \cdots, n). \tag{17}$$

The physical interpretation of this hierarchy of operators acting in the $1, 2, \cdots, n$-particle spaces has often been discussed [10] and we shall not discuss it now. The next theorem establishes some immediate properties of the *g.d.o.*'s.

THEOREM 10. *The pth-order density operator D^p, $p = 1, 2, \cdots, n$, is linear, bounded and self-adjoint operator.*

PROOF. The linearity and boundedness are obvious and one easily shows the self-adjointness by proving that D^p is symmetric (symmetry and boundedness imply self-adjointness), i.e., that $(D^p f_1, f_2) = (f_1, D^p f_2)$ for any two elements $f_1, f_2 \in \mathscr{H}_{(p)}$.

It is often useful to consider in conjunction with D^p, the qth order density operator D^q, with $q = n - p$, defined in the same way as D^p by the kernel

$$D^q(y, y') = \int \Psi(x, y) \overline{\Psi}(x, y')\, dx, \tag{16'}$$

i.e.,

$$D^q g(y) = \int D^q(y, y') g(y')\, dy'$$

$$= \iint \Psi(x, y) \overline{\Psi}(x, y') g(y')\, dx\, dy'. \tag{17'}$$

Obviously, D^q is also linear, bounded and self-adjoint.

THEOREM 11. *The* pth *and* qth *order density operators* D^p, D^q, $(p = 1, 2, \cdots, n - 1)$ *have the product decomposition:*

$$D^p = T_q{}^p \bar{T}_p{}^q = T_q{}^p (T_q{}^p)^* \tag{18}$$

$$D^q = T_p{}^q \bar{T}_q{}^p = T_p{}^q (T_p{}^q)^*. \tag{18'}$$

PROOF. Since $\bar{T}_p{}^q$ is an operator of domain $\mathscr{H}_{(p)}$ and range in $\mathscr{H}_{(q)}$, $\bar{T}_p{}^q f$ is an element of $\mathscr{H}_{(q)}$; $T_q{}^p$ having $\mathscr{H}_{(q)}$ for domain and range in $\mathscr{H}_{(p)}$, the composite mapping $T_q{}^p \bar{T}_p{}^q$ has a meaning and is equal to D^p because both of these operators, as integral operators, are determined by the same kernel. The second part of (18) follows from Theorem 9.

Theorem 11 could serve as an alternate definition of the D^p's; here we shall use it primarily to obtain very directly further properties of the g.d.o.'s but the reader should already be alerted to the interesting computational features of operator decompositions of the form TT^*, as illustrated, e.g., by the works of Kato [11] and others.

THEOREM 12. *The density operators* D^p *and* D^q $(p = 1, 2, \cdots, n - 1)$ *are cc; furthermore, they belong to the trace class and so also to the Schmidt class.*

PROOF. The complete continuity results directly from the product decomposition (18) and the complete continuity of the T's. They belong to the trace class because they are the products of two operators of the Schmidt class (Corollary 2. of Theorem 6).

COROLLARIES

(i) *The D^p's and D^q's admit a (unique) polar representation*

$$D^p = \sum_i \lambda_i^p(\varphi_i^{(p)} \otimes \bar{\varphi}_i^{(p)}) \tag{19}$$

$$D^q = \sum_i \lambda_i^q(\varphi_i^{(q)} \otimes \bar{\varphi}_i^{(q)}). \tag{19'}$$

The λ_i^p's, (λ_i^q's) are the nonzero, real proper values of D^p, (D^q); they are at most of finite multiplicity and form a sequence converging to zero if infinite. The φ_i^p's, (φ_i^q's) are the associated proper functions of D^p, (D^q); they form an o.n. set in $\mathscr{H}_{(p)}$, ($\mathscr{H}_{(q)}$) which is complete iff 0 is not a proper value.

PROOF. By direct application of Theorem 5 since we have established that the D^p's are both *cc* and symmetric.

(ii) *The kernels $D^p(x, x')$ and $D^p(y, y')$ have the representations*

$$D^p(x, x') = \sum_i \lambda_i^p \varphi_i^{(p)}(x)\, \bar{\varphi}_i^{(p)}(x') \tag{20}$$

$$D^q(y, y') = \sum_i \lambda_i^q \varphi_i^{(q)}(y)\, \bar{\varphi}_i^{(q)}(y'), \tag{20'}$$

where the λ's and φ's have the above properties.

THEOREM 13 (Duality). *The* pth *and* qth *order density operators, D^p and D^q, have the same nonzero proper values with the same (finite) multiplicity, the* ith *one being given by:*

$$\lambda_i^p \equiv \lambda_i^q \equiv \lambda_i = \mu_i^2, \tag{21}$$

where μ_i is the ith *proper value of $[T_p{}^q]$ or $[T_q{}^p]$. The proper functions $\varphi_i^{(p)}$ and $\varphi_i^{(q)}$ satisfy the duality relations:*

$$\begin{aligned} T_p{}^q\bar{\varphi}_i^{(p)} &= \mu_i\varphi_i^{(q)} \\ T_q{}^p\bar{\varphi}_i^{(q)} &= \mu_i\varphi_i^{(p)}. \end{aligned} \tag{22}$$

PROOF. It follows directly from the product decomposition (18) and the properties of the Ψ-mappings given earlier since one has then, in addition to (21):

$$\varphi_i^{(p)} = f_i^p \qquad \varphi_i^{(q)} = g_i^q. \tag{23}$$

Indeed, (18), (11′), (14) give

$$D^p f = T_q^{\ p}(T_q^{p*} f) = T_q^{\ p}\left[\sum_i \mu_i (f, f_i^{(p)})\, \bar{g}_i^{(q)}\right]$$

$$= \sum_{ij} \mu_i \mu_j (f, f_i^{(p)})\, (\bar{g}_i^{(q)}, \bar{g}_j^{(q)})\, f_j^{(p)}$$

$$= \sum_i \mu_i^2 (f, f_i^{(p)})\, f_i^{(p)},$$

hence

$$D^p = \sum_i \mu_i^2 (f_i^{(p)} \otimes f_i^{(p)}) \qquad \text{q.e.d.}$$

(Similar proof for D^q.)

THEOREM 14. *The* nth *order density operator* D^n, *defined by the kernel* $\Psi(x)\,\overline{\Psi}(x')$, *where* $x = (x_1, \cdots, x_n)$, *is the orthogonal projection operator on the* Ψ*-ray in* $\mathscr{H}_{(n)}$, *i.e.*,

$$D^n \Phi = (\Phi, \Psi)\, \Psi \tag{24}$$

or

$$D^n = \Psi \otimes \overline{\Psi}. \tag{24′}$$

It is defined everywhere in $\mathscr{H}_{(n)}$, linear, bounded, self-adjoint and idempotent. It is also positive[7] and of trace 1 (idempotency and trace 1 require normalization to 1 of $\Psi : \| \Psi \| = (\Psi, \Psi) = 1$). The proof of this theorem is immediate (all properties mentioned belong to every projector in a Hilbert space). As will be shown now, the D^p's (and D^q's) possess also all these properties with the exception of the idempotency.

THEOREM 15. The density operators D^p and D^q ($p = 1, 2, \cdots, n-1$) *are positive and are of trace* 1.

PROOF. The positivity follows from (18), since one has then for every $f \in \mathscr{H}_{(p)}$

$$(D^p f, f) = (T_q^{\ p}(T_q^{\ p})^* f, f) = (T_q^{p*} f, T_q^{p*} f) = \| T_q^{p*} f \|^2 \geqslant 0.$$

By definition of the trace of an operator, one has

$$Tr D^p = \sum_i (D^p f_i, f_i) = \sum_i \| T_q^{p*} f_i \|^2 = \| T_q^{\ p} \|_\sigma^2 = \| \Psi \|^2 = 1,$$

since Ψ is assumed normalized to 1.

[7] For a definition of positive and positive definite operators, see Ref. 12, p. 3.

COROLLARIES

(i) *All proper values* $\{\lambda_i^{(p)}\}$ *of* D^p *are* $\geqslant 0$.

(ii) *All diagonal elements of any matrix representation of* D^p *are* $\geqslant 0$.

(iii) *All proper values* $\{\lambda_i^{(p)}\}$ *of* $D^p \leqslant 1$.

(iv) *The sum of the proper values of* D^p *is equal to 1, each* $\lambda_i^{(p)}$ *being counted as many times as its multiplicity.*

$$\sum_i \lambda_i^{(p)} = \| \Psi \|^2 = 1. \tag{25}$$

PROOF.

(i), (ii) are direct consequences of the positivity of D^p.

(iii) follows from (iv) and the fact that all $\lambda_i^{(p)}$'s are $\geqslant 0$.

(iv) is a well-known property of the trace of an operator and can be obtained directly from the definition of the trace by taking as c.o.n. set, the set of all proper functions of D^p.

One should note that Theorem 15 implies that the D^p's are symmetric (part of the definition of positivity) and also *cc* because of:

THEOREM 16. *Every positive operator of finite trace is cc.* (A direct proof of this theorem is easily constructed.)

An essential problem in the g.d.o. theory is the so-called representability problem, i.e., the problem of obtaining a *complete* characterization of the D^p's. An answer to this question requires obtaining necessary and sufficient conditions on an operator on $\mathscr{H}_{(p)}$ such that they will ensure the existence of at least one n-particle wave function Ψ from which the tentative density operator can be derived according to the definition of D^p.

If the state space of the system is $\mathscr{H}_{(n)}$, the representability problem is answered by the next theorem; but, of course, such a state space corresponds only to a system of n distinguishable particles; the representability problem for systems of identical particles will be considered in the following papers.

THEOREM 17. *Every positive operator of trace 1 on* $\mathscr{H}_{(p)}$ *is a* pth *order density operator, derivable from an element* $\Psi(x, y)$ *in* $\mathscr{H}_{(n)}$ *and conversely.*

PROOF. Theorem (16) ensures the *cc* of the tentative density operator; it is also symmetric (part of the definition of positivity), so it admits the polar representation (Theorem 5)

$$\sum_i \lambda_i (\varphi_i^{(p)} \otimes \bar{\varphi}_i^{(p)})$$

with

$$\sum_i \lambda_i = 1 \qquad \text{(trace 1)}$$

(the $\varphi_i^{(p)}$'s being o.n. in $\mathscr{H}_{(p)}$).

Consider now the expression

$$\sum_i \sqrt{\lambda_i}\, g_i^{(q)}(y)\, \varphi_i^{p}(x),$$

where $\{g_i^{(q)}\}$ is any o.n. set in $\mathscr{H}_{(q)}$, it is clear that this expression defines an element $\Psi(x, y)$ of $\mathscr{H}_{(n)}$ and one verifies immediately that the associated pth order density operator D^p is the given operator. This shows that the conditions given are sufficient and the converse was established in Theorem 15.

The reader will recognize this last theorem as the equivalent for the g.d.o.'s of the von Neumann theorem on the characterization of a statistical operator.

6. Summary and Conclusions

We have shown that the principal properties of the generalized density operators are direct consequences of those of completely continuous operators induced by the wave function Ψ. By using the appropriate function spaces together with their associated operators we are able to systematically organize the important theorems from which we extract the structure of the density operators in a simple and transparent manner. It is to be noted that the cross operator which was used so effectively in deriving the properties of the density operators and their kernels should not be regarded as just another formal operator introduced as a mathematical convenience. Indeed, it is a reflection of the tensor product nature of $\mathscr{H}_{(n)}$ resulting from $\mathscr{H}_{(p)}$ and $\mathscr{H}_{(q)}$. The kernel representation theorem is likewise a reflection of this same fact as is the duality theorem. These features will be clarified in later papers after we have discussed tensor algebras on a Hilbert space.

The introduction of the Schmidt and trace norms and the fact that finite rank operators, defined on the Banach spaces generated by these norms, lie dense in these spaces will permit us to introduce the methods of functional analysis and therefore to construct bona fide approximation procedures (with resulting *a priori* error estimates) for quantum mechanical calculations. In this way we will gain both geometrical and physical insight into many-body problems.

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